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Methods for Matrix Inversion and for the Solution of Simultaneous Linear Algebraic Equations

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J. H. CURTISS

PREFACE AND SUMMARY OF THE TEXT

TECHNICAL REPORT I

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METHODS FOR MATRIX INVERSION AND FOR THE SOLUTION OF SIMULTANEOUS LINEAR ALGEBRAIC EQUATIONS*

by

J. H. Curtiss

mar. 1954 23 pp

Preface and summary of the text.

Note: The purpose of this technical report is to provide information about a longer work now in rough draft form, with the idea of determining processing requirements and obtaining suggestions for improvement.

(Contracts Nos. DA-30-069-ORD-1257 ;
and
Contract N6ori-201) Task Order No. 1

* Technical Report No. 1

This report represents results obtained at the Institute of Mathematical Sciences, New York University, under the sponsorship of the Army Office of Ordnance Research and the Office of Naval Research.

New York, 1954

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PREFACE.

Professor J. J. Schoenberg once remarked in a lecture at the Institute for Numerical Analysis in Los Angeles that there were two kinds of problems studied in the theory of numerical analysis: problems which do exist, and problems which do not exist. He was of course referring to the pure mathematician's criterion as to the existence of a problem. The problems which do not exist, from this viewpoint, are those for which theorems are available which guarantee solutions under certain circumstances. The theorems may not give any clue as to how to find solutions in practice. The class of problem which do exist is simply defined to be the complement of the class which do not, with respect to the field of numerical analysis.

The inversion of matrices and the solution of systems of linear algebraic equations are problems which most emphatically do not exist, in the above sense. Perhaps the linear equation problem ceased to exist more than three thousand years ago, because one mathematical historian* has traced Cramer's rule in a simple form back to the Chinese of 1100 B.C. Certainly after Cramer (1704-1752), there could be no coubt about the matter.

Cramer's rule not only furnishes an existence theorem; it furnishes a formula for finding solutions numerically. Yet the

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* David Eugene Smith, History of Mathematics, Boston 1923-25. Vol. 2, p. 433.

formula is almost useless in practice unless the order of the matrix of the problem is very low. Forsythe* has recently estimated that to solve 26 equations in 26 unknowns by the use of Cramer's rule and by the definition of determinant would take a modern large-scale electronic computing machine some 10^{17} years. By the most efficient methods, the solution could be reached on the same machine in about 3 seconds of computing time.

It is not surprising, therefore, that an enormous literature concerned with the development of methods of matrix inversion and solving linear equations has come into being. During just the last fifty years, many hundreds of research papers have appeared on the subject. There were numerous contributions in the nineteenth century, also. Good surveys of the literature are now available**. Yet it would seem that there is as yet no exposition in print in the English language which systematically and carefully covers the entire field, both from the point of view of practice and from that of theory. The nearest approach will be found in the interesting new book by A. S. Householder entitled Principles of Numerical Analysis***. But this seems to be written for the teacher and researcher rather than for the novice and the laboratory worker. It is entirely theoretical and contains very few hints as to how to apply the theory.

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* Forsythe, G. E., "Solving Linear Equations Can be Interesting." Bull. Am. Math. Soc., Vol. 59 (1953) pp. 299-329.

** See e.g. Forsythe, loc. cit.

*** New York, 1953.

It was the author's aim to fill this gap, by providing an up-to-date exposition which emphasizes practice, but which also is self-contained as to theory, and which covers all (or nearly all) of the successful and popular methods. A good many more were included which are largely of theoretical interest, with the idea of making the collection useful for research workers.

The presentation has been arranged with a rather particular educational schedule in mind. It is the author's feeling that universities and colleges with programs in numerical analysis should give two years of post-calculus instruction in the subject. The first year should cover the classical topics: interpolation, quadrature, solution of ordinary differential equations, solution of non-linear single equations, and so forth. The second year might well start with matrix inversion and the solution of simultaneous linear equations. It would proceed then to eigenvalues of matrices, and would then go back and apply eigenvalue theory to the important problem of round-off error analysis in linear computation and to other special problems in matrix inversion. Then would follow integral equations, and a long study of partial differential and partial difference equations.

The present work is intended as a reference (or even as a text-book) for the first topic of the second year. Since this topic precedes eigenvalues in the above schedule, they are mentioned in the text only superficially, and no essential developments are made to rest on them. But eigenvalues have not been completely avoided. It is not bad pedagogical practice to antici-

pate future topics, so the author has not hesitated to introduce the definition of eigenvalues in Chapter 1, together with the interesting Geršgorin Theorem, and to make some slight use of the canonical decomposition and the Geršgorin Theorem in Chapter 7.

One boundary condition which the author has imposed on himself is the principle that classroom work in numerical analysis should always be accompanied by laboratory sessions. This in turn means that the students must have something worthwhile and relevant to do in the laboratory sessions. Therefore the theory has been presented on a pay-as-you-go basis, with not much more given at one time than is immediately necessary as a background for the next group of methods. The exception lies in the first chapter, where the prerequisite framework of algebraic theory is quickly erected. It is suggested that the first laboratory session can profitably be devoted to numerical practice in performing matrix iterations and other manipulations.

Each new method is presented first as a cook-book recipe, and then the special theory is developed. The author has hopes that this approach will make the presentation useful as a laboratory manual in addition to its intended service in education and research. Once the basic notation is understood, the instructions given for each method can be followed without any reference to, or understanding of, the theory.

An attempt was made to provide neat and appropriate proofs for the theory sections. Sophisticated geometric methods, and arguments employing the language of abstract spaces, were generally

avoided. This resulted in a substantial reworking of a good portion of the standard theory -- a fact which will be particularly evident to the reader in the treatment of iterative methods. There are a number of apparently new results in Chapters 6 - 8.

It was found that the avoidance of eigenvalue arguments caused negligible difficulty in presenting the theory. On the other hand, it did make the presentation seriously incomplete in one respect: an adequate discussion of round-off error and condition of matrices was necessarily considered to be outside the scope of the work. There may be some external justification for this, in that an adequate theory of error analyses is as yet non-existent for many of the methods presented. The author hopes to return to the subject when time permits and supplement this essay with a complete treatment of round-off error.

In view of certain admirable bibliographic studies which have recently been made by Forsythe* and others, no special effort was

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* See the "Tentative Classification of Methods and Bibliography," etc., of Forsythe in Simultaneous Linear Equations and the Determination of Eigenvalues, National Bureau of Standards, Applied Mathematics Series No. 29, Washington, 1953. The user of the present essay is urgently advised to equip himself with the Forsythe bibliography, especially if older collateral references will be used. The older literature of linear computation is shot through with false credit lines and incorrect assumptions of priority. The author is fully aware in making this statement that the present treatment will undoubtedly contain errors of scholarship which will be shown up by future literature researches.

made to attain any sort of bibliographic stature for this exposition. Many of the references are to secondary sources. Some of the citations were chosen mainly to direct the reader to worked-out numerical examples. The few references to primary sources are either to very new work or to classical work for which the author felt the priority should be emphasized. Foreign language references were largely avoided, again with the idea of making the presentation useful for laboratory technicians*.

The idea for this work grew out of lectures which the author gave at Harvard during the spring term of 1953. He is deeply grateful to Professor Howard Aiken and Dean J. H. Van Vleck for this opportunity.

The Harvard lectures were guided by a set of mimeographed notes of lectures given by G. E. Forsythe at the University of California at Los Angeles in 1951. (The notes were written up by D. G. Aronson and K. E. Iverson .)

The final treatment has strayed rather far from the Harvard lectures. The organization and preparation of the manuscript, and the development of practically all of the new material, was carried out at the Institute of Mathematical Sciences of New York University in the academic year 1953 - 1954, with the support of the Office of Ordnance Research and of the Office of Naval Research.

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* This has the somewhat unfortunate result of excluding detailed references to the excellent and comprehensive expository work of E. Bodewig. It is adequately covered by Forsythe (loc. cit.) however.

SUMMARY OF THE CHAPTERS.

Preliminary Note on Notation.

Capital letters denote n x n real matrices, with the exception that $\dot{X}$, X_o, X_1, ..., and Y are real n x m matrices. Vectors are denoted by Greek letters. The central problem under study is to solve the equation $AX = Y$ for X, given A and Y , where A is real and non-singular. Special cases are the problems $A\xi = \eta$ and $AX = I$. The first of these is the standard simultaneous linear equation problem and the second is the matrix inversion problem .

CHAPTER 1. BACKGROUND

This is an introductory chapter. The primary purpose of the chapter is to make the report largely self-contained as to matrix theory. The central theorem is the reduction of a matrix to what Birkhoff and MacLane call the"echelon form". From this are derived the conditions for non-singularity, and the basic facts about determinants and linear dependence. The chapter also contains a section on operational counts, with a table showing the number of multiplications required to carry out various typical linear computations. There is a section on the relation of matrix inversion to solving linear equations. The importance of a suitable correspondance between equations and unknowns is stressed.

Note: In presenting each of the methods for matrix inversion and for the solution of linear equations in Chapters 2 - 8, the following outline is followed:

(a) Procedure. (Simple instructions to the computer as to what to do, without explanations.)

(b) Modifications. (Variants of (a)).

(c) Checks.

(d) Theory.

(e) Amount of work. (Measured as the nominal number of multiplications required in worst cases.)

(f) References,

CHAPTER 2. ELIMINATION METHODS

Section 2.1. Elimination methods in general. (Contains a general theorem which covers all elimination methods.)

Section 2.2. METHOD I. The Gauss Elimination Method. Four versions are given, with check and theory of check. There is a detailed count of multiplications, with a table giving the numbers of multiplications required to solve various different problems.

Section 2.3. METHOD II. The Complete Elimination Method.

Section 2.4. METHOD III. The Triangular Factorization (Cholesky-Crout) Method. Three versions are given. The second one is the Aiken "below-the-line" variant using an augmented matrix, and the third is the "square-root method" for symmetric matrices. In the Theory, the LDU theorem and its various corollaries are stated and proved. The rpoof used is similar to that of Fadeeva, Computational methods of linear algebra (Russian), Moscow-Leningrad, 1950 in the Forsythe-Benster translation.

CHAPTER 3. ORTHOGONALIZATION

Section 3.1. Positive definite matrices. The main properties of positive definite matrices are stated and proved. It is shown that positive definiteness is invariant under congruence, and is related to the dominant diagonal property. The basic theorem is proved by means of the LDU theorem and not by means of the canonical form.

Section 3.2. S - orthogonality. Definition and properties of S - orthogonal vectors and matrices.

Section 3.3. The Gram-Schmidt Process. The process is developed for S - orthogonalization rather than for I - orthogonalization. The steps and formulas are ultimately exhibited in a table.

Section 3.4. METHOD IV. The Classical Orthogonalization Method. The theory sub-section relates the procedure to elimination procedures and the LDU theorem.

Section 3.5. METHOD V. The Method of Conjugate Directions. Two versions are given. The first is essentially the suggestion of Fox-Huskey-Williamson for symmetric matrices. The second is applicable to general matrices, and is derived from a method of conjugate gradients proposed by E. J. Craig in correspondence with the author*.

Section 3.6. Connections between the orthogonalization methods, and relationships with other methods.

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* New.

Section 3.7. Orthogonal reduction to triple diagonal form. The possibility of using for matrix inversion a reduction to triple diagonal form explcited recently by Givens in the eigenvalue problem is pointed out, but details of the construction are not given.

CHAPTER 4. BLOCK INVERSION AND ESCALATOR METHODS.

Section 4.1 The general formulas for block inversion. The Schur formulas are stated and proved.

Section 4.2. METHOD VI. The Escalator Method. The Morris Escalator Method and its generalization to block steps is stated. The effect of row interchanges to "dodge" a collapse of the method is discussed.

CHAPTER 5. VARIATIONAL FORMULAS

Section 5.1. The inverse of a modified matrix. A general formula is proved for Δ_X, where Δ_X is given by $(A + \Delta_A)(X + \Delta_X) = Y + \Delta_Y$. Various special cases are stated.

Section 5.2. Derivatives and infinitesimals. Partial derivatives of the elements of X with respect to those of A and Y are developed, where X is given by AX = Y. The proofs of the required limit relations do not use Cramer's rule and the theory of functions of many variables*.

Section 5.3. The condition of a matrix. A qualitative treatment that introduces several proposed condition numbers.

Section 5.4. METHOD VII. The method of variation. How to invert a matrix by changing one row or one element at a time in a matrix A_o whose inverse is known.

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* New, but probably unimportant.

CHAPTER 6. DESCENT METHODS

Section 6.1. Iterative methods in general. Distinction between direct and iterative methods; definitions of convergence, residual matrix, error matrix, descent method "step". Properties shared by all good iterative methods. Table of basic recursion relations.

Section 6.2. Elementary theory of descent methods. Proof of equivalence of the three limiting relations $X_N \dashrightarrow A^{-1}Y$, $R_N \dashrightarrow 0$, and $R_N'SR_N \dashrightarrow 0$, where X_N is the N-th approximation in an iterative solution of $AX = Y$, R_N is the N-th residual matrix, and S is any positive definite matrix*. A sufficient condition for convergence of descent methods is stated and proved**. Table of quadratic forms useful in descent methods.

Section 6.3. METHOD VIII. The Relaxation Method. Simplest procedure; group operations; over-relaxing and under-relaxing; various numerical suggestions. In the theory, proof of convergence is given for the case $A > 0$. It is worth noting that by using the results established in Section 6.2, the proof is reduced to two lines, which is in contrast with certain treatments elsewhere in the literature.

Section 6.4. Optimum - a_N methods. The "best" value of a_N in the

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* The method of proof used in connection with $R_N'SR_N$ is probably new; it does not use canonical forms.

** New.

recursion relation $\xi_{N+1} = \xi_N - a_N\delta_N$ for the problem $A\xi = \eta$ is derived. A one parameter modification is developed. A general sufficient condition for the convergence of any modified optimum - a_N method is stated and proved*. It is shown that both the Relaxation Method and the Method of Conjugate Directions are both optimum - a_N methods.

Section 6.5. METHOD IX. The Method of Steepest Descent. The simplest optimum gradient method with a one-parameter modification is described. In the theory, convergence is quickly proved** by referring to Section 6.4. Then the geometric principles involved in the entire class of optimum gradient methods are discussed at some length, starting with elementary ideas from calculus and anlytic geometry.

Section 6.6. METHOD X. The Conjugate Gradient Method. The Hestenes-Stiefel method and Craig modification are presented. Formulas for the inverse and determinant are given. Under theory, the basic orthogonality relation are stated but proof is postponed to Section 6.7. The fact that the method is essentially a variant of the Method of Conjugate Directions is proved. The latter method does not a priori admit zero direction vectors, however, and the resulting distinction between the Conjugate Gradient Method and the Method of Conjugate Directions is discussed with some care***.

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* New

** New

*** New but unimportant.

Section 6.7. Proof of the basic theorem in the Conjugate Gradient Method. The Hestenes-Stiefel double-induction proof, with a little more attention to the possibility of a breakdown of the algorithm than they gave.

Section 6.8. A generalization of the Conjugate Gradient Method.* A generalization is stated and proved which contains all the algorithms known to be useful in practice. Specialization to the Modification in Section 6.6 is given. Formulas for the determinant are derived..

Section 6.9. Other optimum- a_N methods. A table summarizes the various other gradient methods which have been proposed. No evaluation is given.

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* New. Presented by title at Yosemite Meeting of the American Mathematical Society in May, 1954. Paper submitted to Mathematical Tables and Other Aids to Computation.

CHAPTER 7. LINEAR ITERATIVE METHODS.

Section 7.1. Measures of magnitude of matrices. Properties of norms are derived from four axioms discussed by Rella at the Oslo Congress in 1936. Sufficient conditions for $A_1 A_2 \ldots A_N \longrightarrow 0$. If $A^N \longrightarrow 0$, then the elements of A^N approach zero with a geometric degree of convergence*. An inequality for $\| A^{-1} \|$ is derived.** Special norms are presented, together with proofs that they satisfy the Rella axioms (A table of special norms and their properties is given.)

Section 7.2. Classification of iterative processes. Consistency, linearity, stationarity. The most general consistent linear process.

Section 7.3. Elementary convergence theory for linear iterative processes. The relationship between Neumann series and linear iterative processes. Necessary and sufficient conditions for the convergence of Neumann series. Various sufficient conditions for the convergence of linear processes, stated in terms of certain norms. An inequality for $\| A^{-1} \|$ in terms of the norms of matrices involved in a convergent linear process.

Section 7.4. Remarks on the selection and use of linear iterative processes. It is pointed out that there are an infinite number of convergent processes for any problem. Linear iterative

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* New. Published by the author with a different proof in a paper appearing in the Journal of Mathematics and Physics for January 1954.

** Probably known previously but in some other form.

processes are generally stable under round-off error (proof given). Various a posteriori tests of a successful choice of an iterative process. Three different computation procedures for any linear iterative process are presented. An arrangement whereby the non-homogeneous recursion relation $X_{N+1} = HX_N + MY$ is replaced by a homogeneous one $Z_{N+1} = KZ_N$ is presented*.

Section 7.5. Rapidity of convergence of linear processes; acceleration devices. Here for the first time the role of the eigenvalues of H in the relation $X_{N+1} = HX_N + MY$ is brought out. The canonical forms and canonical decompositions of H and of H^N are presented without proof in the non-defective case. The Aiken δ^2- process and another simpler acceleration method are derived.

Section 7.6. Optimum one-parameter adjustment of the matrix MA**. Acceleration devices based on the adjustment of the parameter t in the recursion relation $X_{N+1} = (I-tMA)X + tMY$ are described. First a result based on the smallest and largest eigenvalue of MA (assuming real positive eigenvalues) is given. This is a generalization of known results for the Richardson Method (Section 7.8). Then a method (apparently entirely new) based on minimizing $\|I - tMA\|$ is derived and discussed.

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* Maybe new, but unimportant. Published by the author in the Journal of Mathematics and Physics, loc. cit.

** The material in this Section is new. Publication as a research paper is under consideration.

Section 7.7. Linear iterative methods as descent methods. The heart of this section is a theorem* which states that a sufficient condition for the convergence of the process $\xi_{N+1} = H\xi_N + M\eta$ is that a matrix $S > 0$ exists such that the quadratic form $SAM + M'A'SAM$ is positive definite. The invariance of positive definiteness under congruence is exploited to obtain the simpler condition $(M^{-1})' + M^{-1} - A > 0$ for the case $A > 0$.

Section 7.8. METHOD XI. The Correction-by-Residuals (Richardson) Method. The basic procedure and three modifications are given. The first modification is based on the known optimum adjustment of the process in terms of the least and greatest eigenvalue of A. The second one takes $M = tA'$ in the relation $X_{N+1} = (I - MA)X_N + MY$. The third one is a rather complicated optimum non-stationary one discussed by D. Young in various research papers now being published.

Section 7.9. METHOD XII. The Total-Step (Jacobi) Method. The simplest procedure and an optimum one-parameter modification are given. In the theory, convergence is proved for the case of a dominant diagonal.

Section 7.10. METHOD XIII. The Cyclic Single-Step (Gauss-Seidel) Method. The procedure is first stated in its most economical

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* New. Separate publication if time permits.

form. Then a special one-parameter modification is introduced, and the optimum adjustment used by D. Young in his Harvard Thesis is presented. In the theory, convergence is proved for $A > 0$ by a descent argument. (In view of the theorem of Section 7.7, the proof takes two lines, which can be contrasted with the lengthy and complicated proofs in the literature.) The Collatz Theorem about convergence in the case of a dominant diagonal is also stated, and carefully proved. There is an extended discussion of the amount of work required for each of the various arrangements.

CHAPTER 8. MISCELLANEOUS METHODS.

Section 8.1. Linear Improvement Method. This relates to the improvement of the solution of $AX = Y$ by calculating $R_o = Y - AX_o$, solving $AX_1 = R_o$ for X_1, calculating $R_1 = Y - AX_1$, solving $AX_2 = R_1$ for X_2, and so on. A general theory* is given in which the advantages of having an approximate inverse of A to work with are brought out. There is a careful count of operations, from which a recommendation is formulated as to a choice of procedures*..

Section 8.2. METHOD XV. Polynomial iteration method for improving an inverse. A quadratic and a cubic algorithm are both given, together with instruction* for choosing between them. A general theory of polynomial iterative methods is developed which includes these algorithms as special cases. Inequalities for norms useful in predicting the degree of convergence are derived. Under Amount of Work a careful discussion of the problem of selecting the most economical iterative method is given**, together with a table showing the limits of the amount of work for polynomials of degree 2, 3, 4, 5, 6. It is pointed out that under certain circumstances, linear iteration is better than polynomial iteration*.

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* New

** New. An earlier analysis by Ullman in Ann. Math. Stat. Vol. 15 (1949) 453-462, seems to be invalid because it is based on the assumption that N, the number of iterations required to achieve a given accuracy, is a continuous variable rather than a discrete one.

Section 8.3. METHOL XVI. The Monte Carlo Method*. An improved and simplified version of the author's scheme of importance sampling, published in the Journal of Mathematics and Physics for January 1954, is presented. A comparison is given of the amount of work required for a Monte Carlo solution and various deterministic solutions which atart with the same data.

Section 8.4. METHOD XVII. Characteristic Equation Method.

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* New. Material presented at a Symposium on Monte Carlo Methods held at Gainesville, Florida on March 16-18, 1954. Publication intended.

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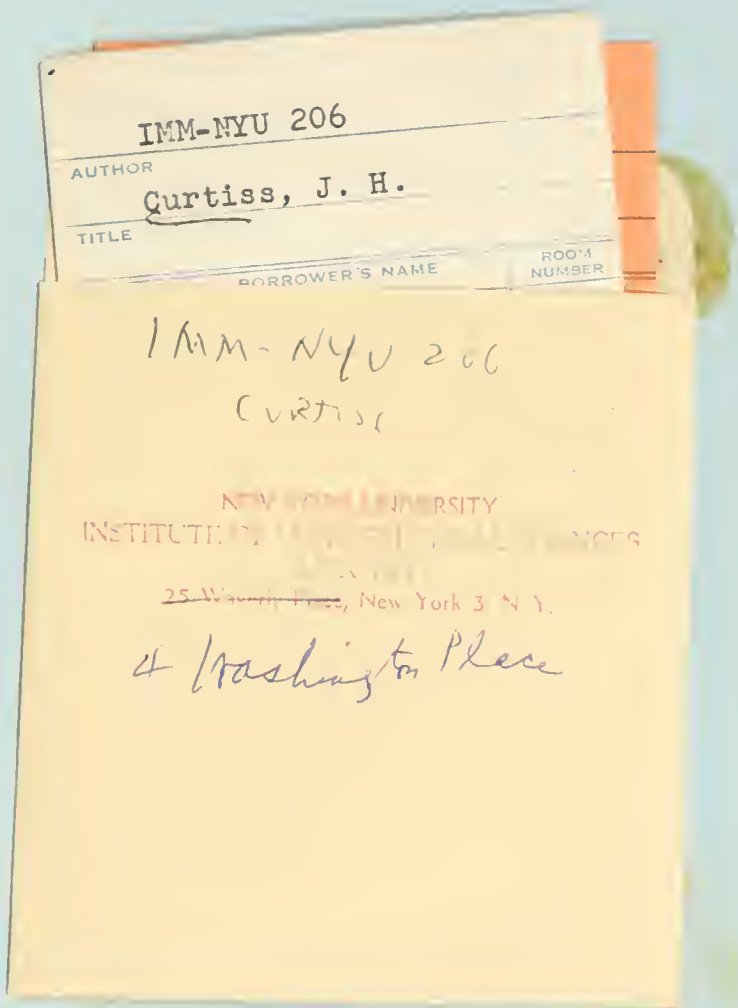

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